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A METHOD OF NUMERICAL INTEGRATION FOR TRANSIENT PROBLEMS OF HEAT CONDUCTION

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Technical Report
to
OFFICE OF NAVAL RESEARCH
Contract N6ori-071(06), Task Order VI
Project NR-064-183

UNIVERSITY OF ILLINOIS
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1. Introduction

In this note, a numerical method of integration is developed for studying transient heat flow in solids. The canonical form of the governing differential equation is of parabolic type, for which various methods of numerical integration have been studied. The present method is more versatile than other methods, and the two methods which give stable solutions, studied by Hyman, Kaplan, and Brien,^{(1)*} are found to be two special cases of the present method.

In the present study, the differential operator with respect to the spatial coordinates is replaced by its eigenvalues. This simplifies the development and the results can be interpreted in terms of eigenmodes of the differential operator, which are found to exist for a great many physical problems, even with time-dependent conditions. A spectrum for the truncational error is obtained with respect to the eigenvalues of the system.

In actual computation the procedure can be either an iterative process, or one which involves solving a set of simultaneous algebraic equations. For the former type of procedure, a criterion for convergence is given; for either procedure, the choice of time interval will

* Numerals in parentheses refer to references similarly numbered in the Bibliography.

have to be limited by a stability criterion. In either case, the continuous spatial differential operator can be either replaced by its finite difference equivalence or converted into a discrete system by the principle of heat balance applied at discrete points.

The type of partial differential equation, which controls the flow of heat in solids, is in fact also that of the governing equation of several physical processes in different engineering fields. For instance, the equation for consolidation of clay, the kinetic equation of rate process, the diffusion equation in chemical reactions, and the Fokker-Planck Equation in the theory of probability, are all of the parabolic type treated in this note.

2. Historical Review

A numerical method of analyzing heat flow in solids was first described by Binder⁽²⁾ and later by Schmidt⁽³⁾ who suggested a graphical method. Their procedure was essentially a step-by-step method without iteration, and the time interval bears a constant ratio to the size of the spatial network. Dusinberre⁽⁴⁾ generalized the procedure by introducing a modulus which releases the restriction in Schmidt's method, but for solids of composite type of different thermal conductivity, odd values of moduli may have to be used. In all these discussions, a simple finite difference was used to replace the derivatives.

Crank and Nicholson⁽⁵⁾ suggested a step-by-step procedure by averaging the time rate of temperature at the two ends of each step in order to get an accurate decrement of temperature in the step. This, however, necessitates the technique of iteration or relaxation for

solving systems of simultaneous algebraic equations for each step of integration, but in general this is not a serious disadvantage to the procedure because of the fact that iteration in a straightforward manner always gives convergent results because of the nature of the matrix of the system. The method discussed in this note is, in fact, a generalization of the above method. Weighting factors are assigned to the time rate of temperature at the two ends of each step, so that in the averaging process an improved decrement can be obtained under various working conditions.

One of the most interesting features of the different numerical procedures is the instability of the numerical solution under certain conditions. Following a method used by von Neumann, Hyman, Kaplan, and Brien⁽¹⁾ studied the stability criterion for different numerical procedures applied to different initial value problems, including the problem of heat conduction. Eddy⁽⁶⁾ also arrived at the same conclusion, but through a different approach. In several of his papers on problems of heat conduction, Fowler⁽⁷⁾ also discussed appropriate ways for preventing unstable numerical solutions.

The method suggested in this note will always yield stable solutions. Moreover, the performance of the procedure is viewed in terms of the modes of the spatial differential or difference operators. The conclusion thus derived is, therefore, independent of the manner in which the Laplacian operator is approximated.

3. β -Method of Numerical Integration

The differential equation of heat flow in solids is usually of the following type

$$\frac{\partial W}{\partial t} = \sum_{ij} \frac{\partial}{\partial x_i} (a_{ij} \frac{\partial W}{\partial x_j}) \quad (1)$$

where W is the temperature in the solid, and the quantities a_{ij} are given functions of time and spatial coordinates. The elementary theory of heat conduction usually deals with a simplified version in which the given functions are constants. In comparison with experimental evidences this is not an unreasonable assumption. The canonical form of the differential equation then can be obtained after a suitable transformation of spatial coordinates, with the result

$$\frac{\partial W}{\partial t} = c \Delta W \quad (2)$$

where c is a constant, and Δ is the Laplace Operator.

In actual computation, the right-hand-side of either Eq. (1) or Eq. (2) can be replaced by a discrete system which may be found by using an equivalent finite-difference scheme for the continuous differential operator. Thus, the right-hand-side can be written as

$$\frac{dW_i}{dt} = \sum_{j=1}^N C_{ij} W_j \quad i = 1 \dots N \quad (3)$$

Hence, the integration of W on the time coordinate can be made by a step-by-step scheme in which the range of time is divided into small

finite steps. For each step, one can make the reasonable assumption that W at the end of each step can be computed by the following formula

$$W_{i,1} = W_{i,0} + h \left[(1 - \beta) \left(\frac{dW_i}{dt} \right)_0 + \beta \left(\frac{dW_i}{dt} \right)_1 \right] \quad (4)$$

where β is a parameter. For most efficient use of the procedure, β should be limited to values between zero and unity.

In Eq. (4), the second subscript 0 refers to the quantities at the beginning of each step, and the second subscript 1, at the end of each step. Equation (4), though empirical in its form, represents a way of computing the change in temperature in a small step of length h due to the temperature rate. If β is taken as $1/2$, it implies that the variation of temperature rate in the small interval is linear. Then

$$W_{i,1} = W_{i,0} + \frac{h}{2} \left[\left(\frac{dW_i}{dt} \right)_0 + \left(\frac{dW_i}{dt} \right)_1 \right] \quad (5)$$

Therefore the iterative procedure can proceed by assuming trial values for temperature rate, dW_i/dt , by which $W_{i,1}$ can be computed from Eq. (5). Then the derived values are substituted back into Eqs. (4) and the new temperature rates, dW_i/dt , are obtained. Repetition of the procedure, with the derived values used as new trial values, is necessary until the difference between the derived and trial values are negligibly small. This can always be achieved if the time interval, h , the length of each step, is properly chosen.

However, if a non-iterative procedure is desired, Eq. (5) can be used to eliminate all $W_{i,1}$ from Eq. (3) and a system of algebraic

equations results,

$$\sum_{j=1}^N (\delta_{ij} - C_{ij} \beta h) \left(\frac{dW_i}{dt} \right)_1 = \sum_j C_{ij} \left[W_{j,o} + (1 - \beta) h \left(\frac{dW_j}{dt} \right)_o \right] \quad (6)$$

The solution of the above system represents the temperature rate at various points at the end of the step, and the temperature, W_1 , can be computed from Eq. (5) accordingly.

Obviously, this scheme will give the distribution of temperature in the solid at any instant under any conditions, including time dependence or temperature dependence for the constants, C_{ij} . In the latter case, Eq. (3) will be non-linear.

4. Convergence and Stability Criteria for the β -Methods

If the right-hand-side of Eq. (1) or Eq. (3) is linear in W , it can be shown that the quantity in the right-hand-side can be replaced by a sum of products of eigenvalues and the corresponding eigen modes with appropriate coefficients, known as Fourier coefficients. Even if time-dependent functions are involved, this principle in a weak sense still can be used in successive short-time intervals during each of which the functions are tentatively assumed as constants. The property that

$$\sum_j C_{ij} y_j^{(n)} = - \lambda_n y_i^{(n)} \quad (7)$$

where λ_n is an eigenvalue and $y_i^{(n)}$ is the corresponding eigenvector, can simplify the mathematical manipulation a great deal since Eq. (3)

can then be written as

$$\frac{dz_i}{dt} = \lambda_i z_i \quad (8)$$

where z_i being the unknowns, are the Fourier coefficients in the representation of W in the form

$$W_i = \sum_j z_j y_i^{(j)} \quad (9)$$

For most of the physical problems of heat conduction, it can be shown that λ_i is always positive. Various methods of numerical integration may be scrutinized with regard to their merit in producing accurate results for each mode separately.

Using Eq. (4) for z , i.e.

$$z_{i,1} = z_{i,0} + h \left[(1 - \beta) \left(\frac{dz_i}{dt} \right)_0 + \beta \left(\frac{dz_i}{dt} \right)_1 \right] \quad (10)$$

one can arrive at the following difference equation by substituting Eq. (8) for dz_i/dt in the above equation.

$$z_{i,n} (1 + \beta \lambda h) - z_{i,n-1} \left[1 - \lambda h (1 - \beta) \right] = 0 \quad (11)$$

The solution to this difference equation can be found easily by assuming that

$$z_{i,n} = C_i (\alpha_i)^n$$

whence

$$\alpha_i = \frac{1 - \lambda_i h(1 - \beta)}{1 + \beta \lambda_i h}$$

and the solution is

$$z_{i,n} = z_{i,0} \left[\frac{1 - \lambda_i h(1 - \beta)}{1 + \beta \lambda_i h} \right]^n \quad (12)$$

where $z_{i,0}$ is the initial value of z_i . The exact solution of Eq. (8) is simply

$$z_i = z_{i,0} \exp(-\lambda_i t) = z_{i,0} \exp(-n\lambda_i h) \quad (13)$$

Physically there is expected a monotonically decreasing solution as time increases. However, this can be achieved if one chooses the parameters β and h in such a way that

$$0 < \frac{1 - \lambda h(1 - \beta)}{1 + \beta \lambda h} < 1 \quad (14)$$

If the lower bound is not satisfied, oscillation begins to appear after a few steps of integration. But, in fact, this oscillation will not cause serious concern if the amplitude does not build itself up. As long as the following relation is satisfied,

$$-1 < \frac{1 - \lambda h(1 - \beta)}{1 + \beta \lambda h} < 1 \quad (15)$$

the residual oscillation will attenuate into insignificance and will not impair the accuracy of the solution. If the above condition is not satisfied, this residual oscillation will continue with an ever increasing amplitude, and after several steps of integration the practical significance of the numerical solution will be completely perturbed by the erroneous higher modes which normally should not share any importance in most problems of heat conduction.

After further simplification, the criterion for stability can be stated as

$$0 < \lambda h < \frac{2}{1 - 2\beta} \quad (16)$$

This partly agrees with the result obtained by Brien, Hyman, and Kaplan⁽¹⁾, since the procedure for $\beta = 1/2$ is exactly their unconditionally stable procedure, in which the Laplacian was replaced by the mean of finite-difference representations at two ends of the time-mesh.

Although (16) is not explicitly clear for β taking on values greater than $1/2$, the optimum range as considered in the present paper, the following study of (15) shows that the ratio

$$\frac{1 - \lambda h (1 - \beta)}{1 + \beta \lambda h}$$

will never have the chance to be algebraically less than -1 for the optimum range of β , between $1/2$ and 1 .

It can be shown that the lower bound of (16) is satisfied if one can restrict the values of β and h to satisfy the following inequality.

$$\frac{\lambda h}{1 + \beta \lambda h} < 2$$

After rearranging the numerator and denominator, one obtains another version of the inequality.

$$\frac{\frac{1}{\beta}}{\frac{1}{\beta \lambda h} + 1} < 2$$

Clearly this requirement can be met for any choice of time interval if β is chosen greater than $1/2$.

Nevertheless if an oscillation-free solution is desired, as it should be, a stringent criterion is obtained by setting the lower bound of (15) as zero, which leads to the result:

$$\lambda h < \frac{1}{1 - \beta} \quad (17)$$

If the procedure is carried out on iterative basis, a criterion for convergence of the procedure is suggested for the choice of time interval in order to give a satisfactory result. If one denotes $z'_{n,0}$ as the trial temperature rate at the end of n -th step, then the derived temperature is, according to Eq. (10)

$$z_{n,1} = z_{n-1} + h \left[z'_{n-1}(1 - \beta) + \beta z'_{n,0} \right] = C + \beta h z'_{n,0}$$

where C is a constant containing given initial values. Now substituting this value back in Eq. (8) one obtains the derived temperature rate, $z'_{n,1}$. If the process is repeated, one obtains the second derived temperature rate $z'_{n,2}$ for which the first derived rate is taken as the trial value. Thus

$$z'_{n,1} = C - \lambda \beta h z'_{n,0}$$

$$z'_{n,2} = C - \lambda \beta h z'_{n,1}$$

The difference of these two equations gives

$$\Delta z'_{n,1} = -\lambda \beta h \Delta z'_{n,0} \quad (18)$$

or, after i -th iteration,

$$\frac{\Delta z_{n,i}'}{\Delta z_{n,i-1}'} = -\lambda\beta h$$

If the process converges, one should expect

$$\left| \frac{\Delta z_{n,i}'}{\Delta z_{n,i-1}'} \right| < 1$$

consequently,

$$\lambda\beta h < 1$$

or

$$\lambda h < \frac{1}{\beta} \quad (19)$$

which is the proper criterion for convergence. Hence, from comparison of (19) and (17), it is found that convergence insures stability when β is greater than $1/4$, but when β is less than $1/4$ the converse is true. To be certain that oscillation is eliminated also, convergence insures freedom from oscillation only when β is greater than $1/2$.

5. Truncational Error of the β -Methods

A comparison between Eq. (12) and the exact solution, Eq. (13) will reveal the influence of various values of β on the numerical solution. Since both solutions attenuate as time increases, the rate at which the solution attenuates gives an indication as to how the truncational error influences the final outcome. Figure 1 is a spectrum of the ratio

$$\frac{1 - (1 - \beta)\lambda h}{1 + \beta\lambda h} \exp(\lambda h) \quad (20)$$

with respect to λh , the product of the eigenvalue and the time interval. If the ratio is greater than one, it means the numerical solution decays faster than it should; if it is less than 1, the numerical solution decays more slowly. In both cases the numerical solutions are stable and non-oscillatory. However, if the ratio is negative, it indicates that the numerical solution will oscillate but with diminishing amplitude, providing the time interval has been chosen in compliance with the stability criterion, Eq. (16). In most practical problems this wriggling of higher modes might not be noticeable.

In Fig. 1, it seems neither $\beta = 1$ nor $\beta = 1/2$, although they give stable solutions, will give reasonably good results so far as a wide range of eigenvalues is concerned. The intermediate value, $\beta = 3/4$, seems to be a better selection; this value gives good results for lower modes, a little boost for mid-range, which is not objectionable, and drops at higher modes; there will be small oscillations for higher modes but they will be damped out eventually.

In view of the spectrum, the $\beta = 0$ procedure, the conditionally stable method, studied by Hyman, Kaplan, and Brien⁽¹⁾, is certainly not a good choice, nor is the method for $\beta = 1/2$, even though the latter is stable for all choices of time-interval.

If the eigenvalues of a problem have been given or computed, though this is seldom done, one may be tempted to find a compromise value for β in order to get a reasonable answer with the use of a large

time-interval. By equating Eq. (20) to unity, the critical β that can preserve the rate of decay is found to be

$$\beta_{cr} = \frac{1}{1 - e^{-\lambda h}}$$

A plot of the above expression is shown in Fig. 2, which shows a flat curve with respect to λh . A compromise value of β can be selected if it is known that the eigenvalues are clustered within a narrow band.

For the sake of comparison, a Runge-Kutta Formula of fourth order is applied to Eq. (8), and the equivalent difference scheme is found as

$$z_n = z_0 \left(1 - \lambda h + \frac{\lambda^2 h^2}{2} - \frac{\lambda^3 h^3}{6} + \frac{\lambda^4 h^4}{24} \right)$$

Unfortunately the bracketed quantity becomes greater than unity when $\lambda h > 2.7853$ even though the bracketed quantity is a truncated portion of the series expansion of the exact solution $\exp(-\lambda h)$. This means the Runge-Kutta procedure will result in stable solutions only for small values of the time interval.

In order to check the stability criterion for the $\beta = 0$ procedure, the conditionally stable method of Hyman⁽¹⁾, etc, a three by three matrix is set for the Laplacian, with zero boundary condition at the ends, namely,

$$C_{ij} = \frac{1}{\Delta_x^2} \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}$$

The third eigen mode is $-1/\sqrt{2}$, $+1$, $-1/\sqrt{2}$ which has an eigenvalue, $(2 + \sqrt{2})/\Delta x^2$. According to Eq. (16) the stability criterion for choosing the time interval is

$$\frac{h}{\Delta x^2} < \frac{2}{2 + \sqrt{2}} = 0.5857$$

while the criterion suggested by Hyman, etc,⁽¹⁾ is

$$\frac{h}{\Delta x^2} \leq 0.5$$

which is more stringent than it should be. In fact, Hyman's criterion represents the asymptotic limit as the rank of C_{ij} becomes infinitely large.

6. Illustrative Example

The heat flow in a quenched slab is chosen as an example to show the performance of different methods. The slab with thickness d is assumed heated uniformly at temperature T_0 . Then it is quenched in a fluid of zero temperature. The problem is to find the distribution of temperature in the slab as a function of time. For mathematical expediency, by assuming a unit coefficient of thermal conductivity, one can easily set up the partial differential equation as

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$$

where the x -axis is directed through the depth of the slab. The appropriate boundary conditions are

$$T = 0, \text{ at } x = 0, \text{ and } x = d \text{ for all } t$$

$$T = T_0 \text{ for all } x, \text{ when } t = t_0$$

The exact solution to the problem has been obtained by Carslaw and can be found in most textbooks on heat conduction. Here it will serve as a check.

Having replaced the one-dimensional Laplacian by the equivalent finite difference relation, one obtains a set of ordinary differential equations, as follows,

$$\frac{dT_i}{dt} = \sum_j C_{ij} T_j \quad i, j = 1 \dots N, \quad N = \frac{d}{2\Delta x}$$

$$C_{ij} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & . & . \\ 1 & -2 & 1 & . \\ . & 1 & -2 & 1 \\ . & . & 2 & -2 \end{pmatrix}$$

Both the boundary conditions and the symmetry of the solution have been considered.

The problem was solved by the $\beta = 3/4$ method and the Runge-Kutta Fourth Order method, for the sake of comparison. The length of time interval was taken as 0.0075 which unfortunately threw the Runge-Kutta procedure into the unstable domain. Therefore, 0.005 was also used for the procedure. Figure 3 shows the distribution of temperature in the half-thickness for $t = 0.0075$, as computed by the two procedures. On account of the unstable ninth mode, the Runge-Kutta method does not

show good agreement with the Carslaw solution while the $\beta = 3/4$ method does. In Fig. 4, the distribution of temperature at $t = .015$, the results from the Runge-Kutta procedure are even worse. The trouble caused by the unstable ninth mode in Fig. 5 is obvious in Fig. 5 in which the temperature at the mid-plane of the slab is plotted against the time factor. The unstable Runge-Kutta solution grows wildly after the first few steps while the result from the $\beta = 3/4$ method follows closely the Carslaw solution. However, after the time interval was cut down to 0.005, which gives a stable solution for the Runge-Kutta procedure, the numerical solutions follow the exact solution faithfully, as shown by the circled dots in Fig. 5.

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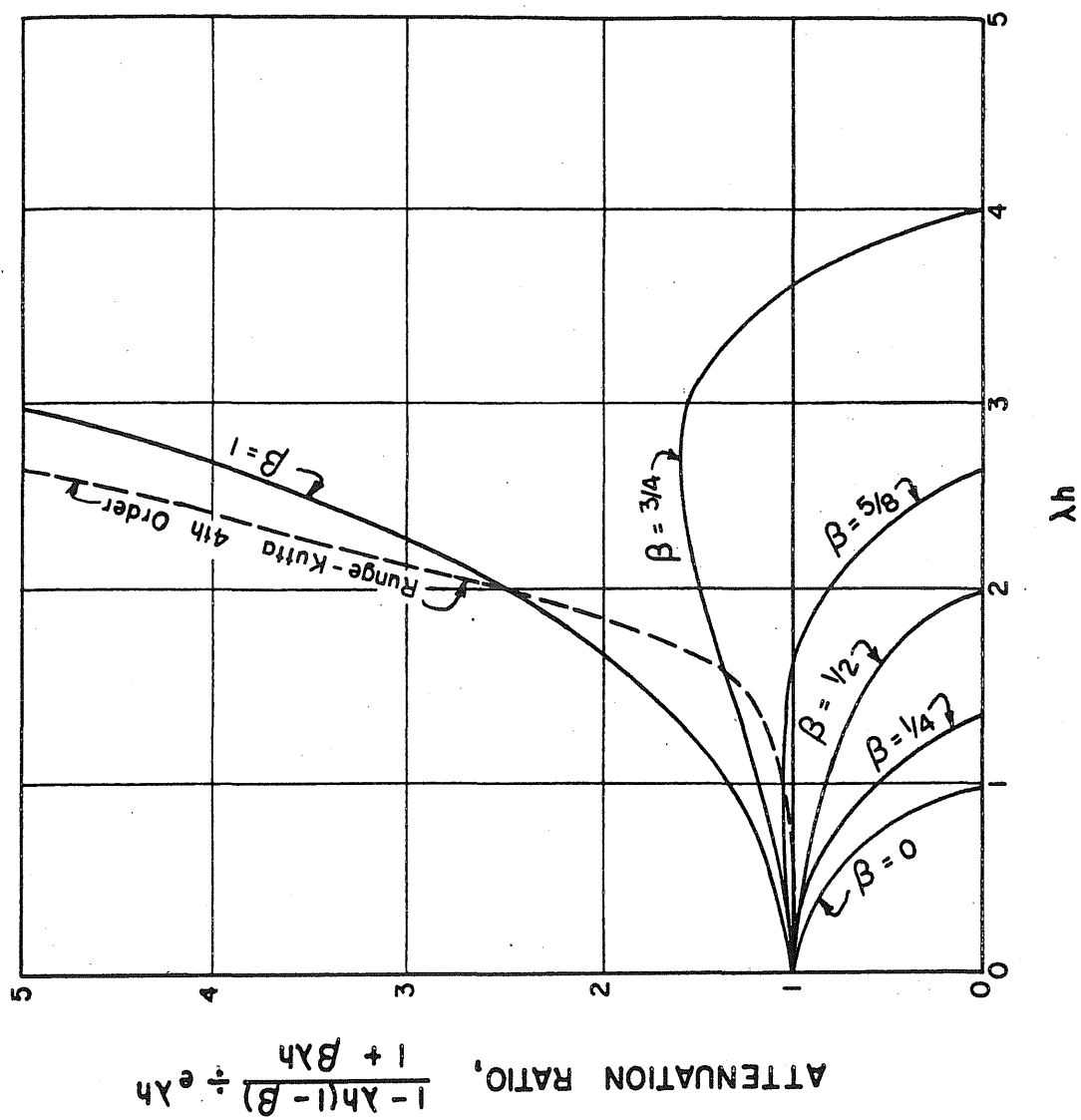


FIG. 1 COMPARISON OF ATTENUATION RATIOS

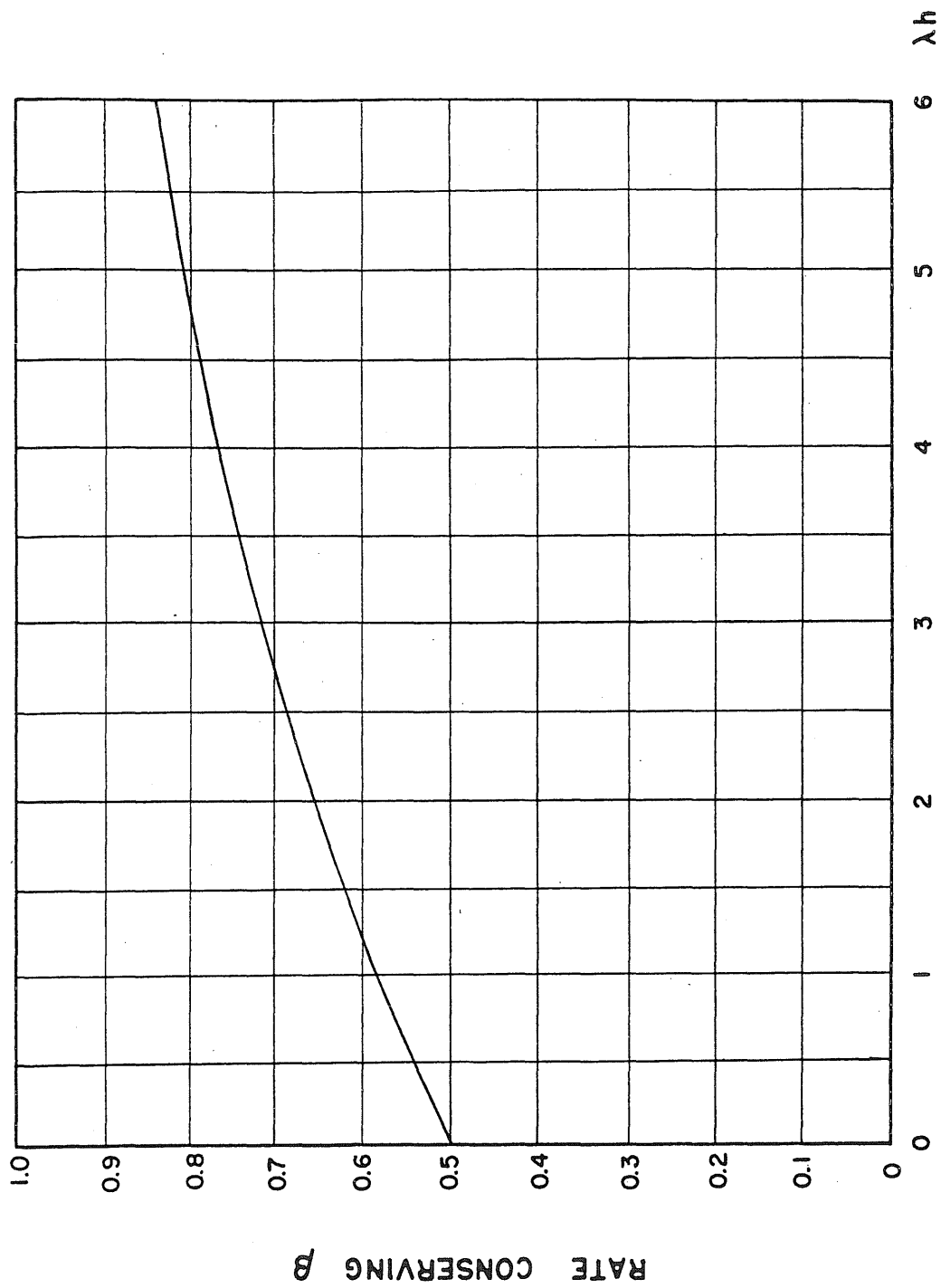


FIG. 2 - β FOR CONSERVING ATTENUATION RATE

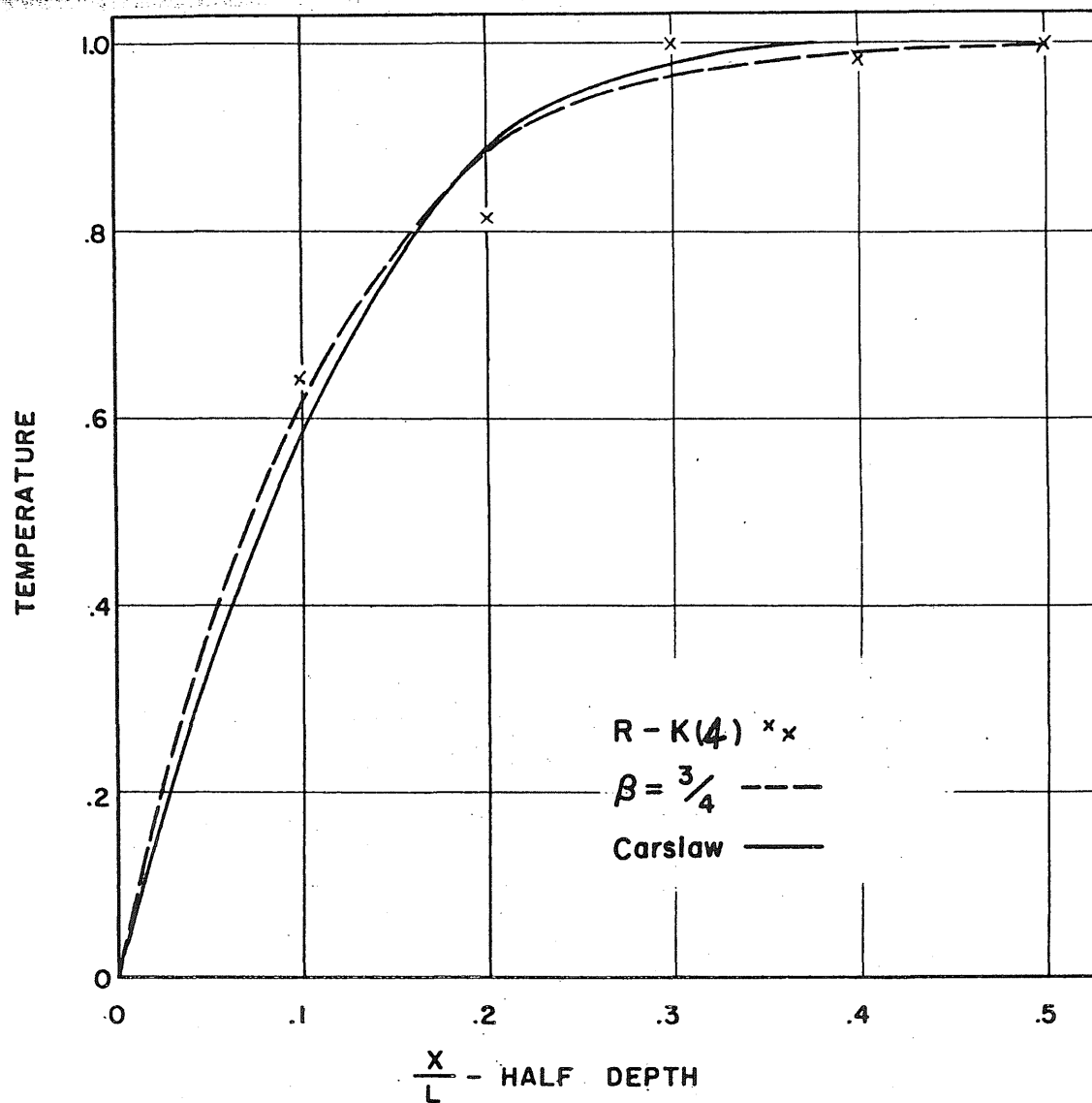


FIG. 3 - DISTRIBUTION OF TEMPERATURE OVER
HALF - DEPTH OF PLATE, AT $t = .0075$

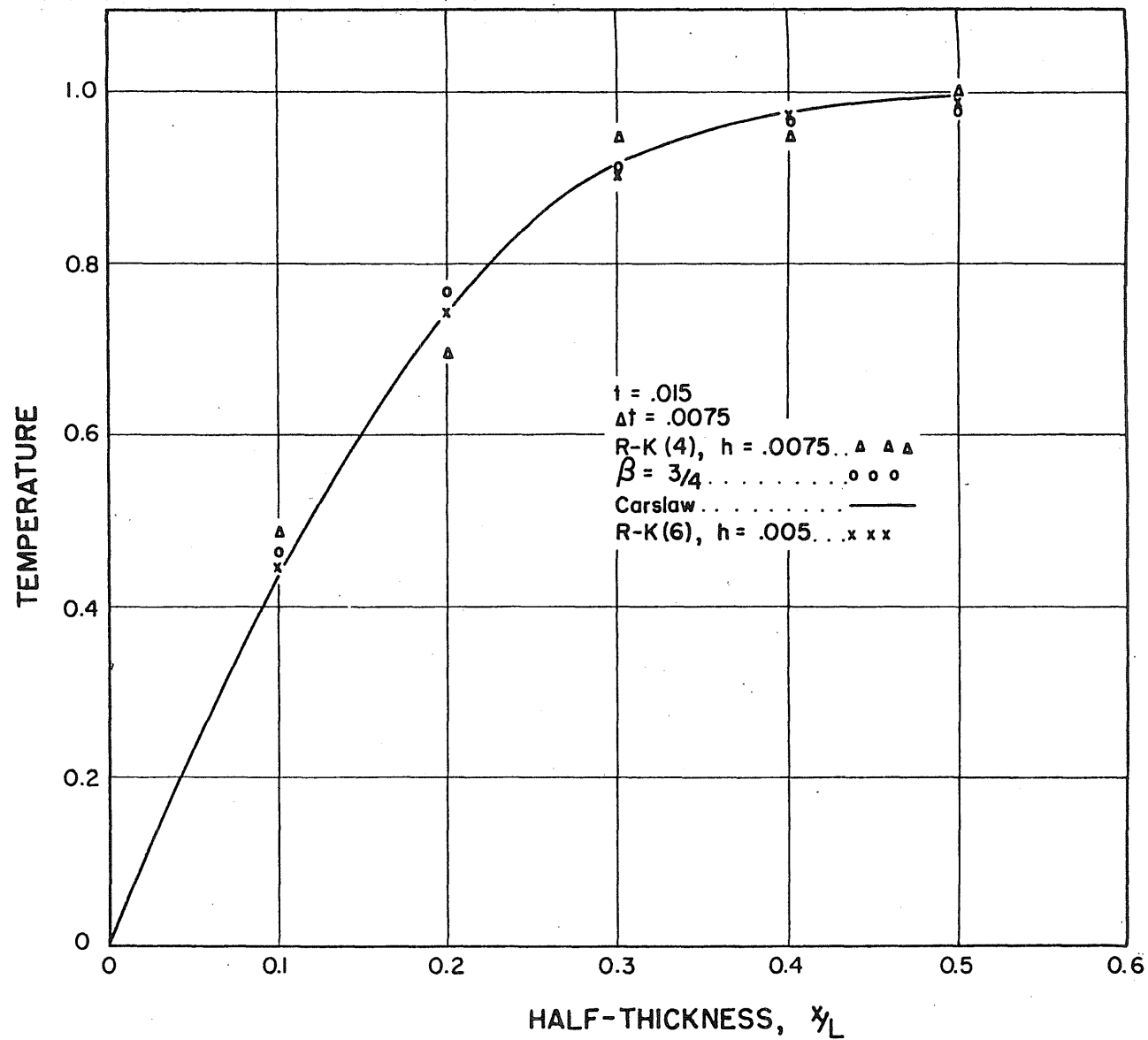


FIG: 4 DISTRIBUTION OF TEMPERATURE OVER HALF-DEPTH AT $t = .015$

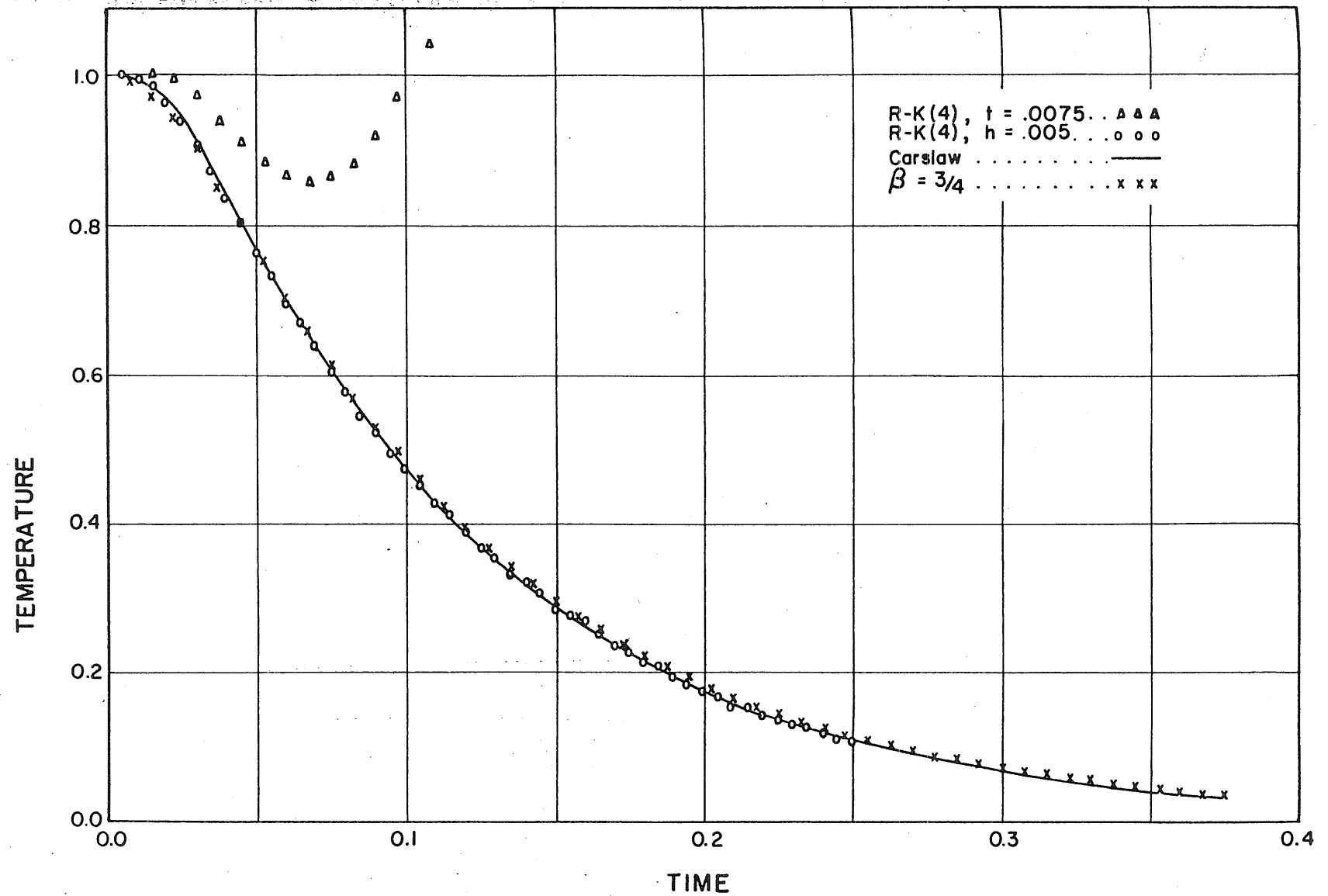


FIG. 5 VARIATION OF TEMPERATURE WITH TIME AT MID-PLANE OF PLATE

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